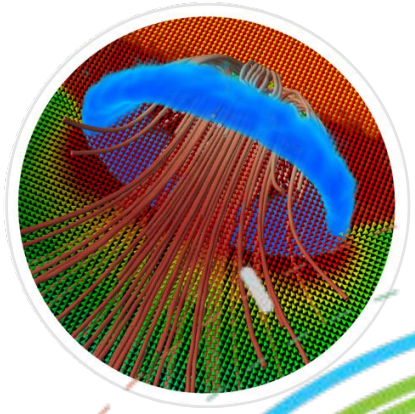
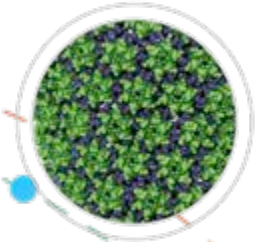
Material and chemistry – vis and applications

Aaron Knoll
SCI Institute, University of Utah



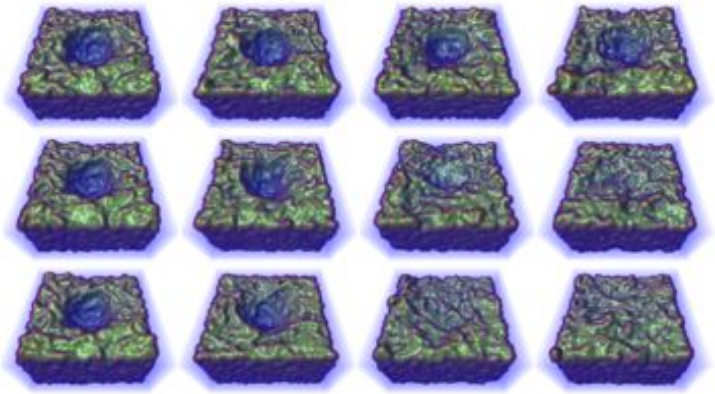


Argonne **Leadership Computing** Facility

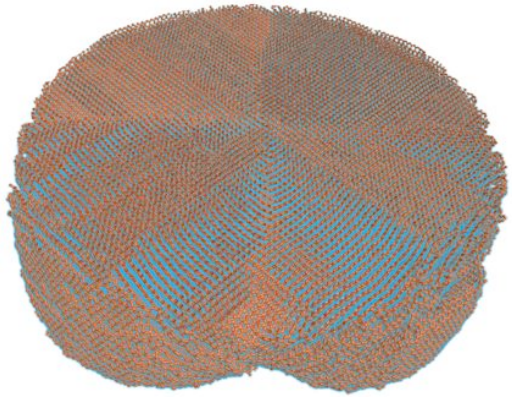
Argonne NATIONAL LABORATORY

Materials and chemistry

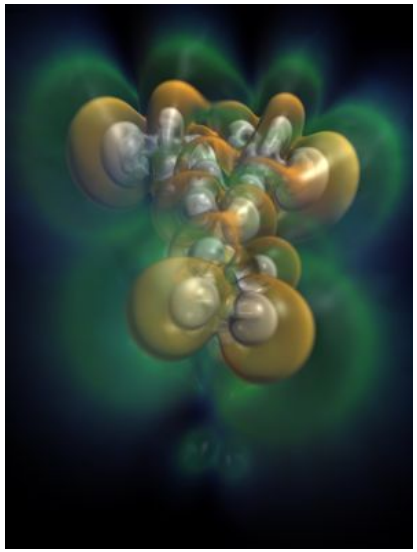
- Energy research is a core mission at ANL
  - Battery, photovoltaics, biofuels, catalysis
  - Not always the largest science, but a large number of jobs
- A different set of tools than “general vis”
  - VMD, Avogadro, Vesta, PyMol, Chimera, Materials Studio
- Larger materials data can be a challenge
  - Volume rendering and analysis
  - “Direct” visualization



Maria Chan, Center for Nanoscale Materials



KC Lau, Materials Science Division



Julius Jellinek, Chemical Science and Engineering

Interaction and immersive environments

- CAVE2 at Electronics Visualization Lab, University of Illinois Chicago

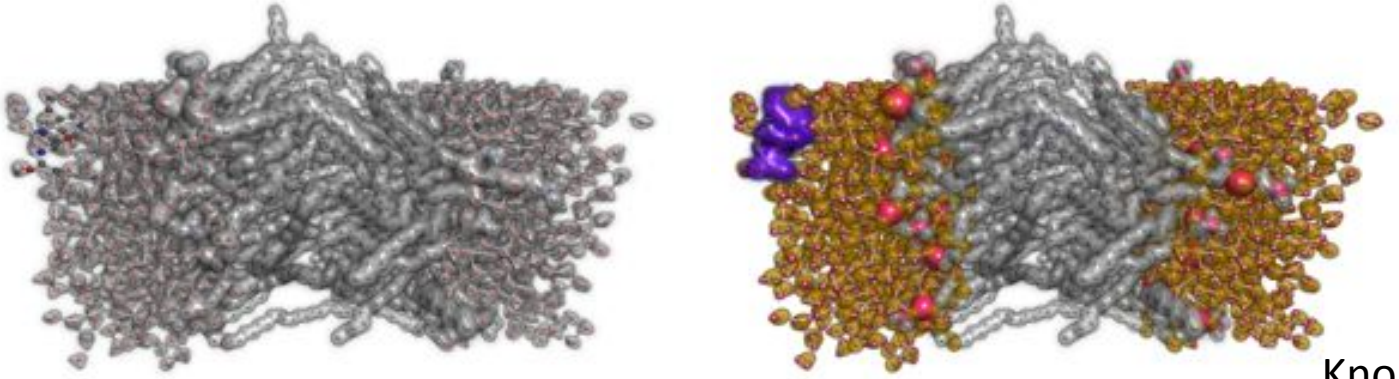
Reda et al. LDAV 2013

- Streaming a 1 Gigapixel image to Stallion at TACC

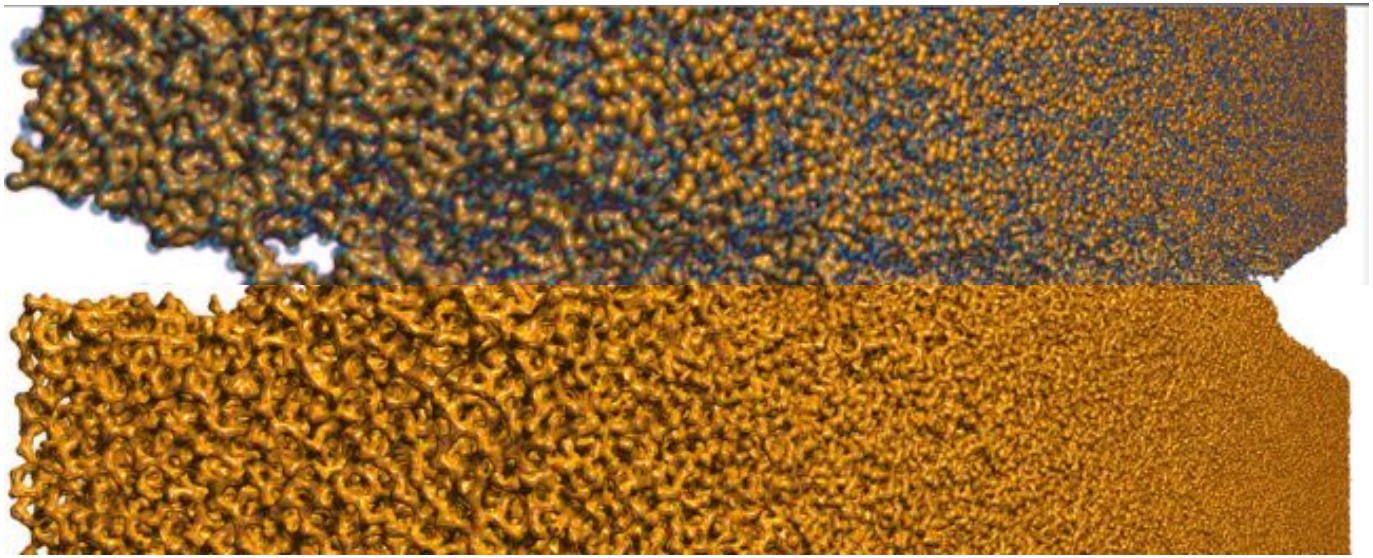
Knoll et al. Ultravis 2013

Direct RBF volume rendering

- No filters, lower memory footprint
- Visualization on CPU or Xeon Phi

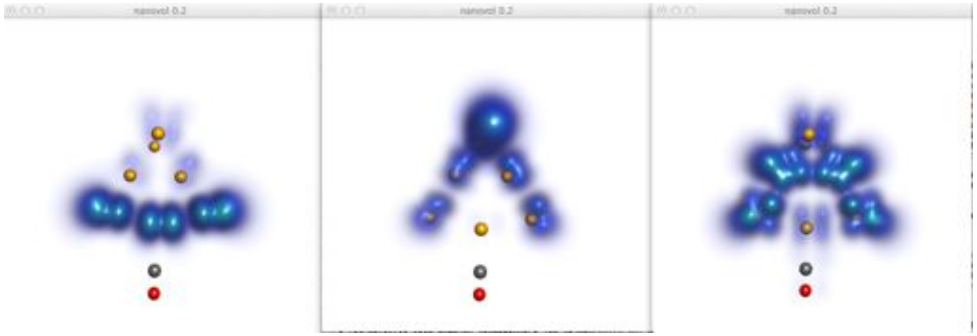


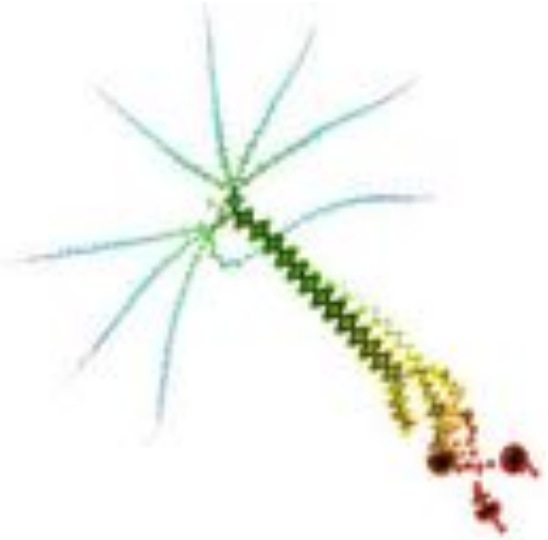
Knoll et al. Eurovis 2014



Analysis

Finding bonds from multifield molecular orbital data
Joint Contour Net (Duke et al. IEEE Vis 2012)





Modeling ion diffusion
Morse Smale Complex (Gyulassy et al. Vis 12)